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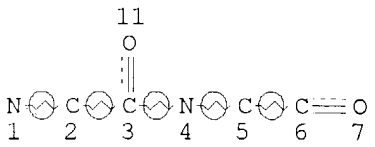
L14 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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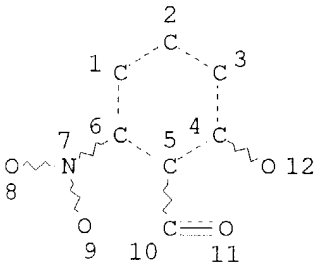
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE
L16 90710 SEA FILE=REGISTRY SSS FUL L14
L18 STR



NODE ATTRIBUTES:
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE
L20 393 SEA FILE=REGISTRY SSS FUL L18
L22 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L16 AND L20

=> d l22 ibib abs hitstr 1-4

L22 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:501665 HCAPLUS
DOCUMENT NUMBER: 139:197756
TITLE: Difficult Macrocyclizations: New Strategies for Synthesizing Highly Strained Cyclic Tetrapeptides
AUTHOR(S): Meutermans, Wim D. F.; Bourne, Gregory T.; Golding, Simon W.; Horton, Douglas A.; Campitelli, Marc R.; Craik, David; Scanlon, Martin; Smythe, Mark L.
CORPORATE SOURCE: Institute for Molecular Bioscience, University of Queensland, St. Lucia, 4072, Australia

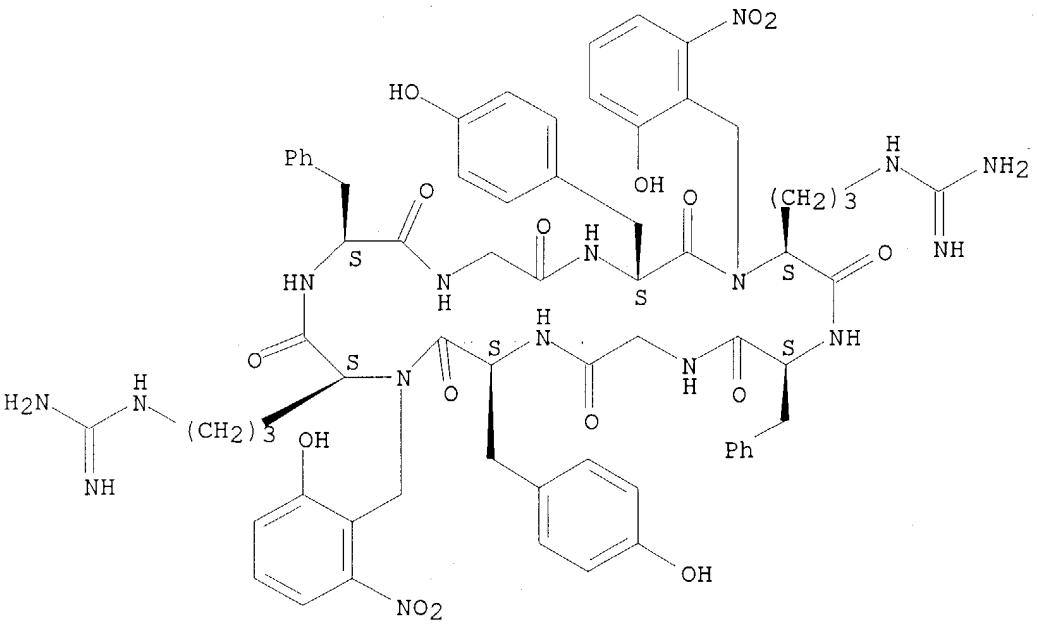
SOURCE: Organic Letters (2003), 5(15), 2711-2714
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:197756

AB To synthesize highly strained cyclic tetrapeptides, the authors developed a macrocyclization strategy that involves the inclusion of 2-hydroxy-6-nitrobenzyl (HnB) as an N-protective group at the N-terminus and in the "middle" of the sequence. The N-terminal auxiliary performs a ring closure/ring contraction role, and the backbone auxiliary promotes cis amide bonds to facilitate the otherwise difficult ring contraction. Following this route, the all-L cyclo[Tyr-Arg-Phe-Ala] was successfully prepared

IT **583051-34-7P 583051-36-9P**
RL: BYP (Byproduct); PREP (Preparation)
(preparation of highly strained cyclic tetrapeptides via cyclizations of linear peptides containing N-protecting hydroxynitrobenzyl groups)

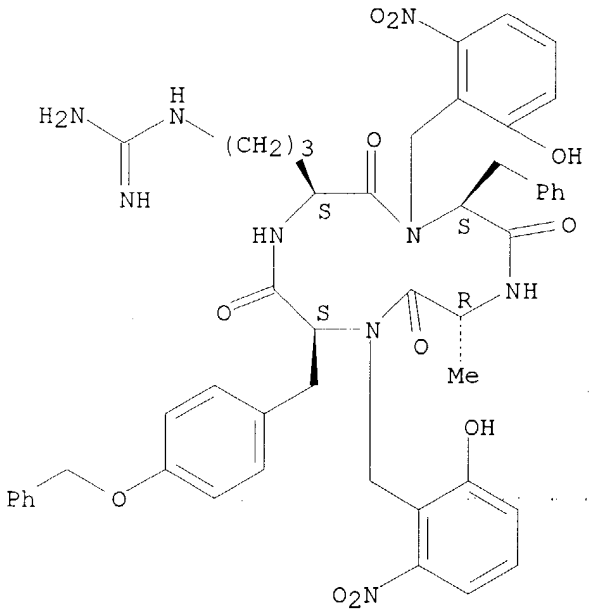
RN 583051-34-7 HCAPLUS
CN Cyclo[N2-[(2-hydroxy-6-nitrophenyl)methyl]-L-arginyl-L-phenylalanylglycyl-L-tyrosyl-N2-[(2-hydroxy-6-nitrophenyl)methyl]-L-arginyl-L-phenylalanylglycyl-L-tyrosyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

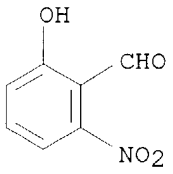


RN 583051-36-9 HCAPLUS
CN Cyclo[D-alanyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-O-(phenylmethyl)-L-tyrosyl-L-arginyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-L-phenylalanyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



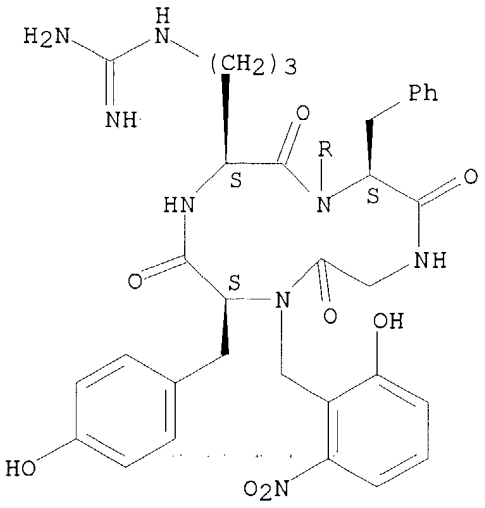
IT **16855-08-6**, 2-Hydroxy-6-nitrobenzaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of highly strained cyclic tetrapeptides via cyclizations of linear peptides containing N-protecting hydroxynitrobenzyl groups)
RN 16855-08-6 HCAPLUS
CN Benzaldehyde, 2-hydroxy-6-nitro- (9CI) (CA INDEX NAME)



IT **263276-96-6P 263277-01-6P 263277-08-3P 263277-33-4P 583051-15-4P 583051-37-0P 583051-38-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of highly strained cyclic tetrapeptides via cyclizations of linear peptides containing N-protecting hydroxynitrobenzyl groups)
RN 263276-96-6 HCAPLUS
CN Cyclo[L-arginyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-L-phenylalanylglycyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-L-tyrosyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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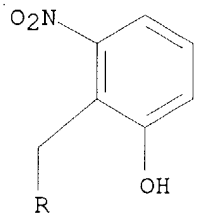
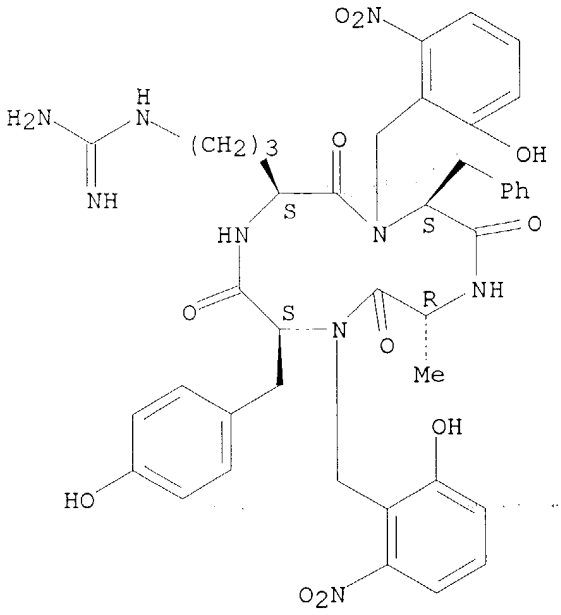


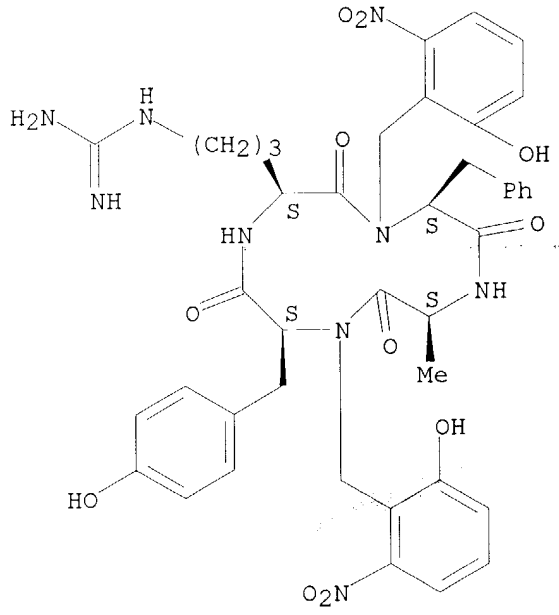
RN 263277-01-6 HCAPLUS
CN Cyclo[D-alanyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-L-tyrosyl-L-arginyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-L-phenylalanyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



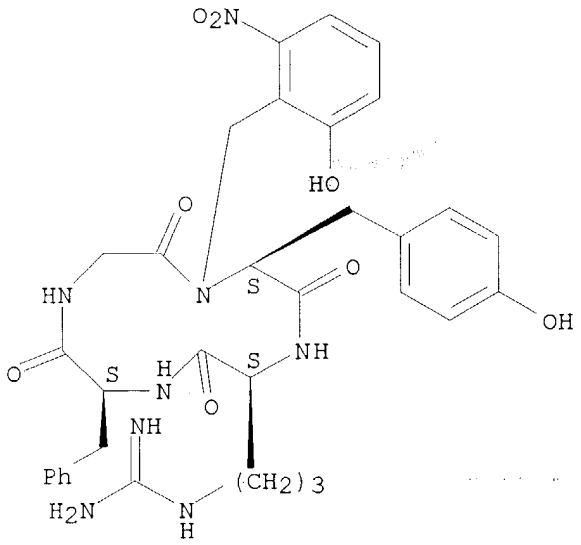
RN 263277-08-3 HCAPLUS
CN Cyclo[L-alanyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-L-tyrosyl-L-arginyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-L-phenylalanyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



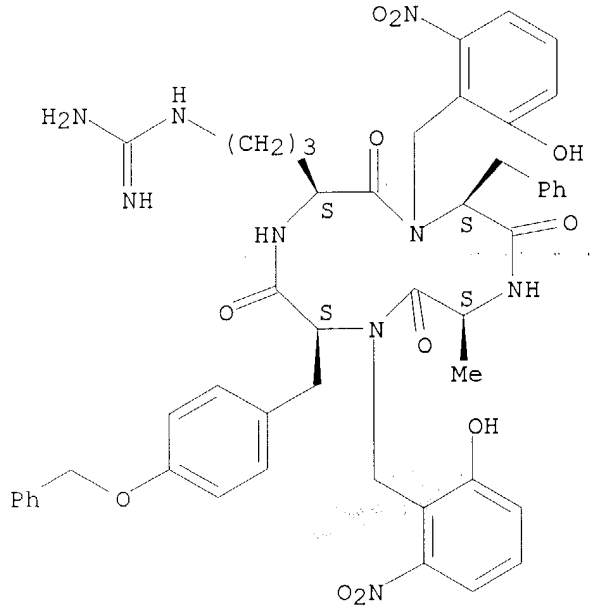
RN 263277-33-4 HCAPLUS
CN Cyclo[L-arginyl-L-phenylalanylglycyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-L-tyrosyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 583051-15-4 HCAPLUS
CN Cyclo[L-alanyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-O-(phenylmethyl)-L-tyrosyl-L-arginyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-L-phenylalanyl] (9CI) (CA INDEX NAME)

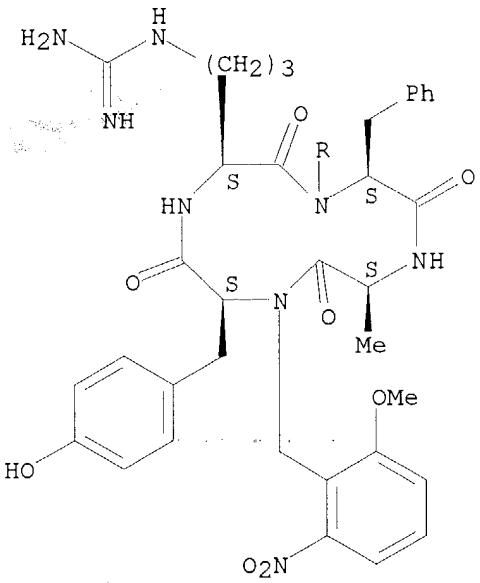
Absolute stereochemistry.



RN 583051-37-0 HCAPLUS
CN Cyclo[L-alanyl-N-[(2-methoxy-6-nitrophenyl)methyl]-L-tyrosyl-L-arginyl-N-[(2-methoxy-6-nitrophenyl)methyl]-L-phenylalanyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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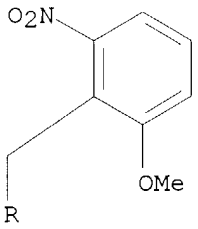
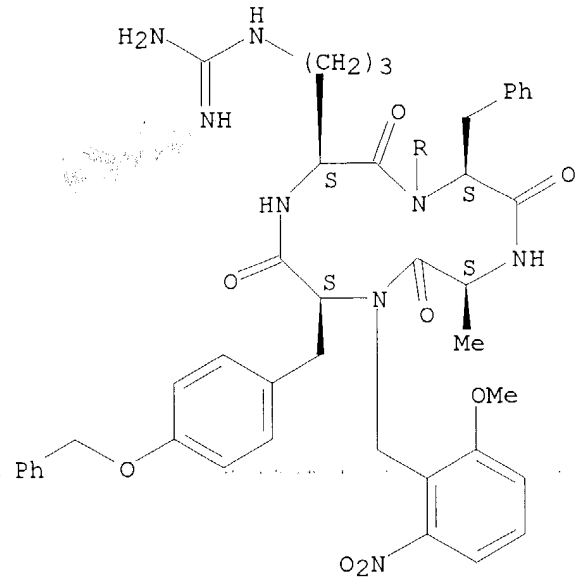


RN 583051-38-1 HCAPLUS
CN Cyclo[L-alanyl-N-[(2-methoxy-6-nitrophenyl)methyl]-O-(phenylmethyl)-L-tyrosyl-L-arginyl-N-[(2-methoxy-6-nitrophenyl)methyl]-L-phenylalanyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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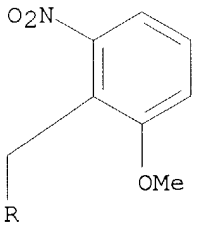
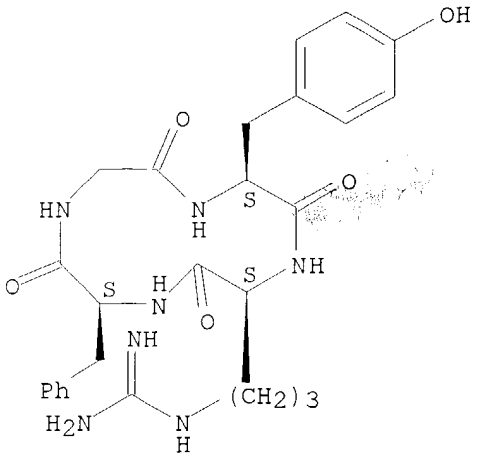


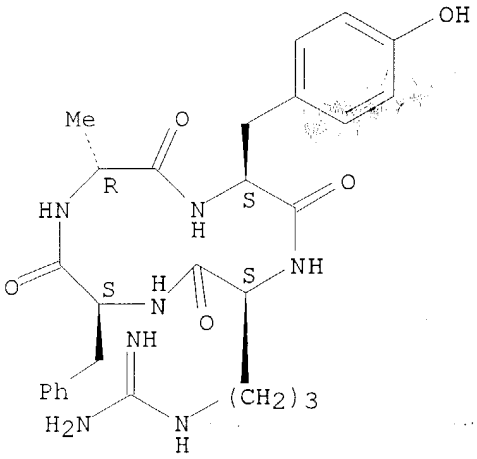
IT **263144-23-6P 263277-02-7P 583051-18-7P**
583051-22-3P 583051-31-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of highly strained cyclic tetrapeptides via cyclizations of linear peptides containing N-protecting hydroxynitrobenzyl groups)
RN 263144-23-6 HCAPLUS
CN Cyclo(L-arginyl-L-phenylalanylglycyl-L-tyrosyl) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



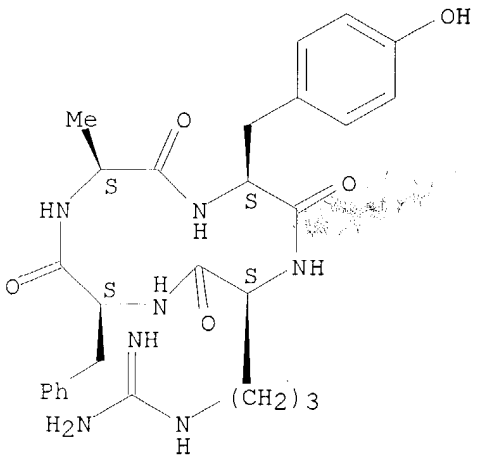
RN 263277-02-7 HCAPLUS
CN Cyclo(D-alanyl-L-tyrosyl-L-arginyl-L-phenylalanyl) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



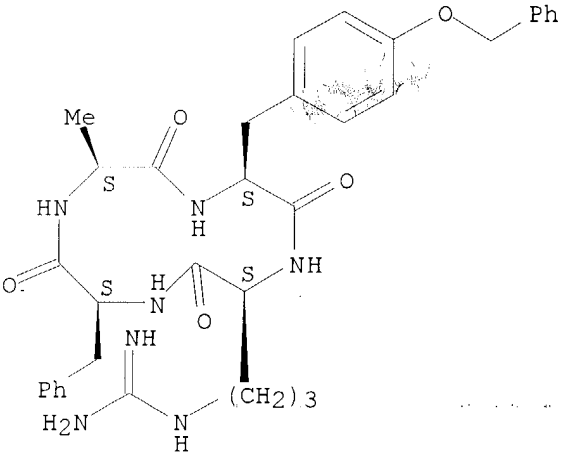
RN 583051-18-7 HCAPLUS
CN Cyclo(L-alanyl-L-tyrosyl-L-arginyl-L-phenylalanyl) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



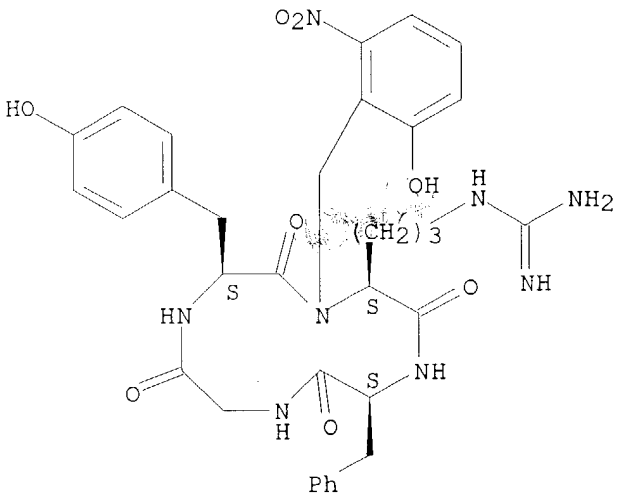
RN 583051-22-3 HCAPLUS
CN Cyclo[L-alanyl-O-(phenylmethyl)-L-tyrosyl-L-arginyl-L-phenylalanyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 583051-31-4 HCAPLUS
CN Cyclo[N2-[(2-hydroxy-6-nitrophenyl)methyl]-L-arginyl-L-phenylalanylglycyl-L-tyrosyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:227674 HCAPLUS
DOCUMENT NUMBER: 132:265505
TITLE: Solid phase synthesis of small cyclic peptides via on-resin cyclization
INVENTOR(S): Smythe, Mark Leslie; Meutermans, Wim Denise Frans
PATENT ASSIGNEE(S): The University of Queensland, Australia
SOURCE: PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000018789	A1	20000406	WO 1999-AU812	19990924
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2345067	AA	20000406	CA 1999-2345067	19990924
AU 9963196	A1	20000417	AU 1999-63196	19990924
AU 768649	B2	20031218		
EP 1115739	A1	20010718	EP 1999-950390	19990924
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002525376	T2	20020813	JP 2000-572247	19990924

PRIORITY APPLN. INFO.: AU 1998-6165 A 19980925
WO 1999-AU812 W 19990924

OTHER SOURCE(S): CASREACT 132:265505; MARPAT 132:265505

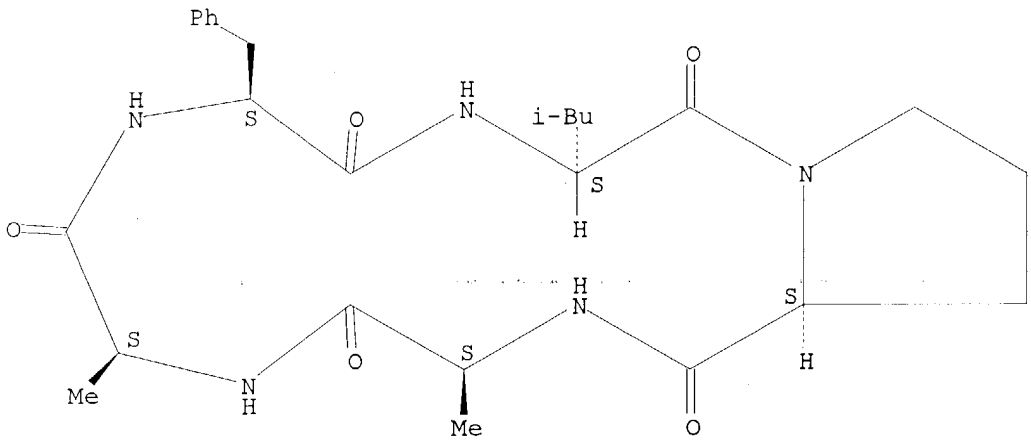
AB This invention relates to novel auxiliaries for the formation of amide bonds, and to the use of these auxiliaries in a variety of synthetic applications, such as the synthesis of peptides and peptidomimetic compds., and in particular for the synthesis of "small cyclic peptides", so-called "difficult" peptide sequences, and large peptides with a native peptide backbone. The auxiliaries of the invention are also useful in the synthesis of peptides or of C-terminal modified peptides, and in on-resin cyclization of organic mols., ligating chemical, backbone substitution and as backbone linkers. In a particularly preferred embodiment, the invention provides auxiliaries which can be removed by photolysis. Methods of synthesis of a linear or cyclic peptide, a C-terminal modified peptide, or of on-resin cyclization of a peptide mol., comprising the step of linking an amine nitrogen atom to an auxiliary compound of the invention, specific auxiliary compds., which may optionally be linked to a solid support, and kits for synthesis are disclosed and claimed. Thus, cyclo-[Ala-Phe-Leu-Pro-Ala] was prepared via on. resin cyclization reaction.

IT **189031-42-3P 263144-21-4P 263144-23-6P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(solid phase synthesis of small cyclic peptides via on-resin cyclization)

RN 189031-42-3 HCAPLUS

CN Cyclo(L-alanyl-L-alanyl-L-phenylalanyl-L-leucyl-L-prolyl) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

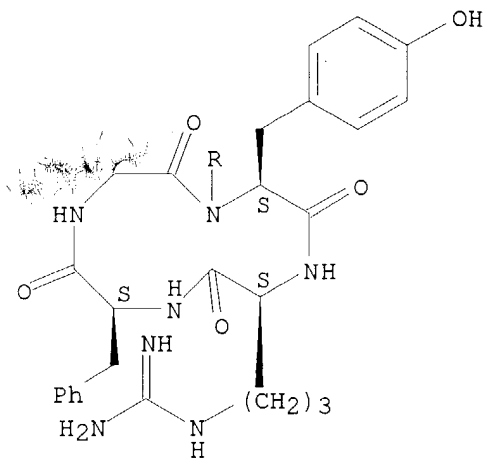


RN 263144-21-4 HCAPLUS

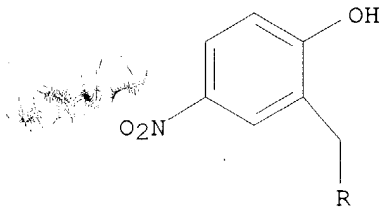
CN Cyclo[L-arginyl-L-phenylalanylglycyl-N-[(2-hydroxy-5-nitrophenyl)methyl]-L-tyrosyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

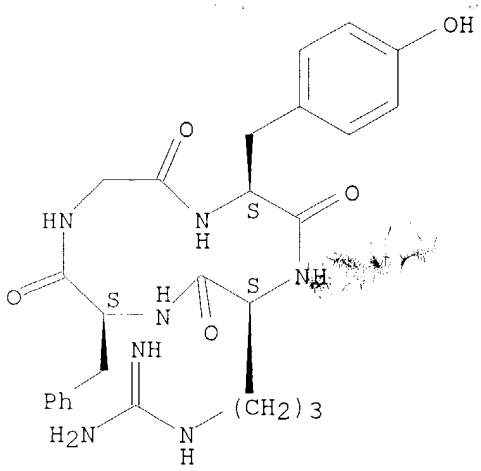


PAGE 2-A



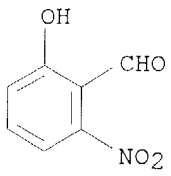
RN 263144-23-6 HCAPLUS
CN Cyclo(L-arginyl-L-phenylalanylglycyl-L-tyrosyl) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **16855-08-6**

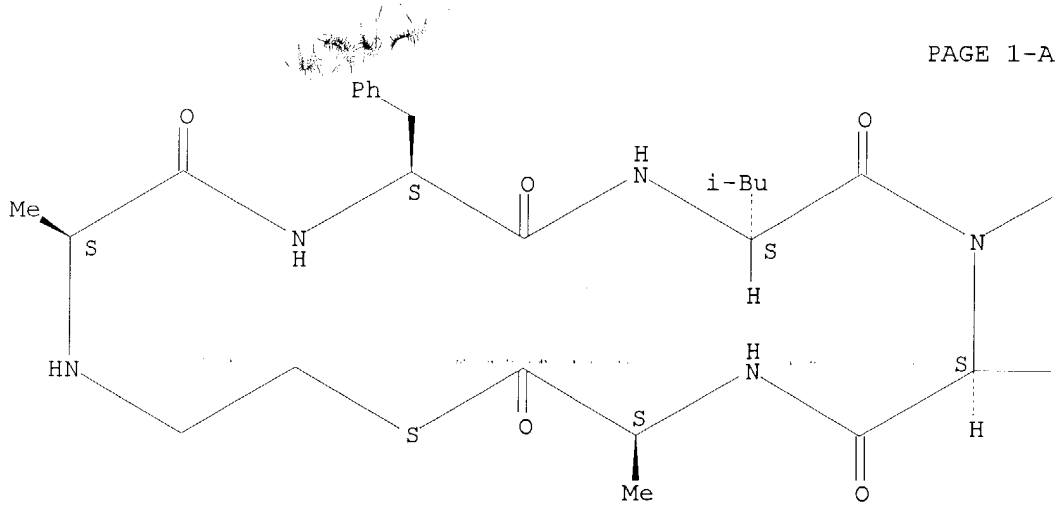
RL: RCT (Reactant); RACT (Reactant or reagent)
(solid phase synthesis of small cyclic peptides via on-resin cyclization)
RN 16855-08-6 HCAPLUS
CN Benzaldehyde, 2-hydroxy-6-nitro- (9CI) (CA INDEX NAME)

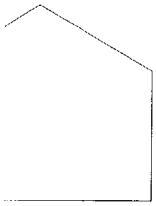


IT **252667-12-2P 252667-14-4P 252667-19-9P 263144-18-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(solid phase synthesis of small cyclic peptides via on-resin cyclization)
RN 252667-12-2 HCAPLUS
CN L-Alanine, N-(2-mercaptoethyl)-L-alanyl-L-phenylalanyl-L-leucyl-L-prolyl-, (5→1)-thiolactone (9CI) (CA INDEX NAME)

Absolute stereochemistry.

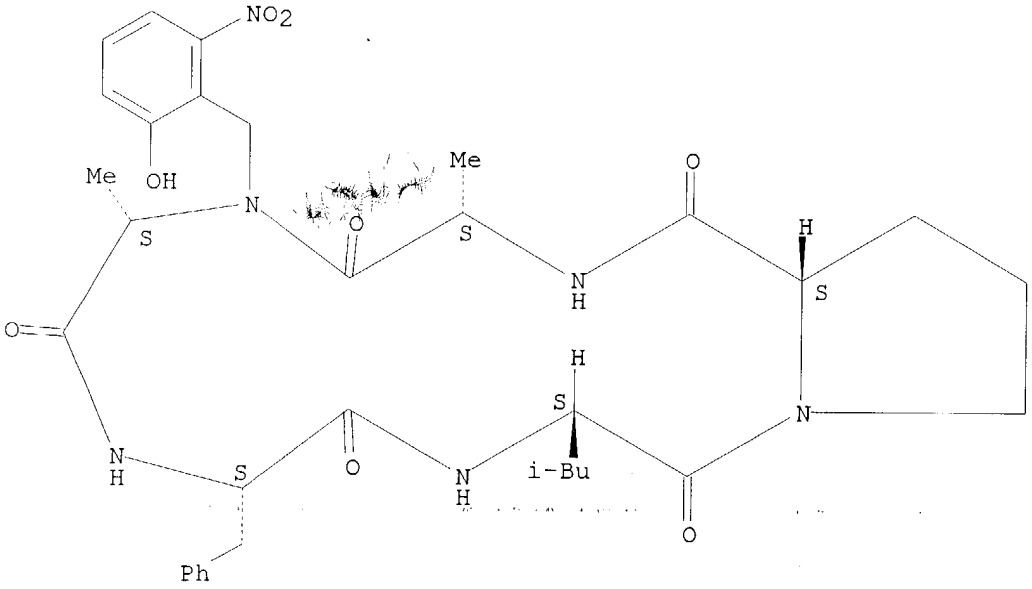
PAGE 1-A





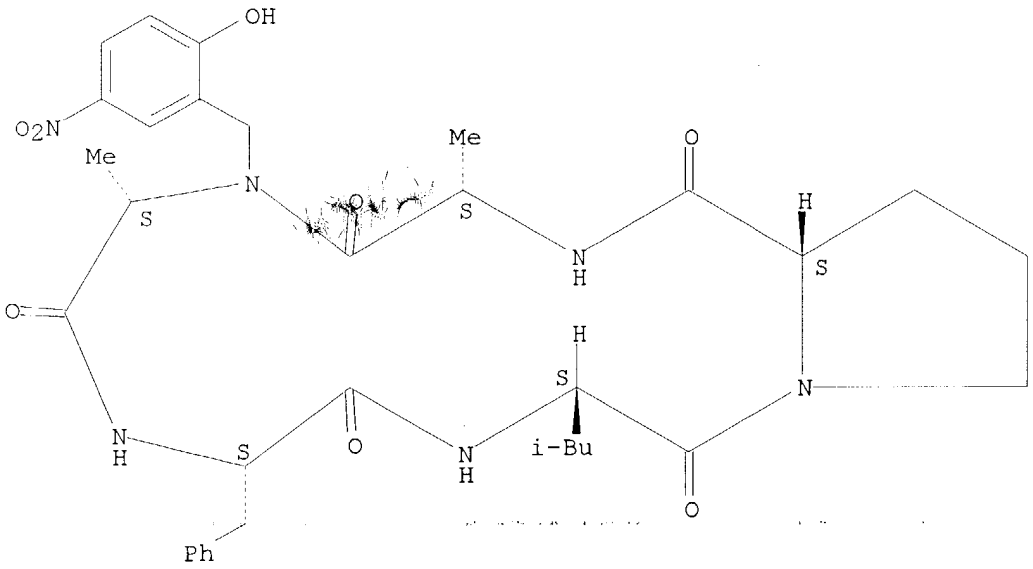
RN 252667-14-4 HCAPLUS
CN Cyclo[L-alanyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-L-alanyl-L-phenylalanyl-L-leucyl-L-prolyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



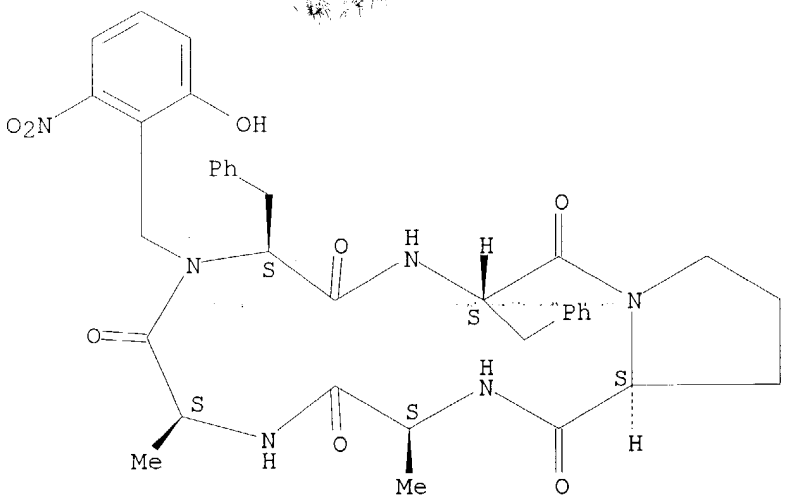
RN 252667-19-9 HCAPLUS
CN Cyclo[L-alanyl-N-[(2-hydroxy-5-nitrophenyl)methyl]-L-alanyl-L-phenylalanyl-L-leucyl-L-prolyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 263144-18-9 HCAPLUS
CN Cyclo[L-alanyl-L-alanyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-L-phenylalanyl-L-phenylalanyl-L-prolyl] (9CI) (CA INDEX NAME)

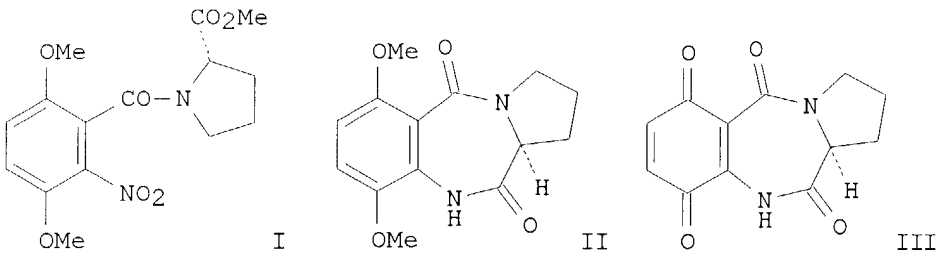
Absolute stereochemistry.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:287131 HCAPLUS
DOCUMENT NUMBER: 131:44797
TITLE: Synthesis of a pyrrolo[1,4]benzodiazepinequinone
AUTHOR(S): Tapia, Ricardo A.; Centella, Cesar R.; Valderrama, Jaime A.
CORPORATE SOURCE: Facultad de Quimica, Pontificia Universidad Catolica

de Chile, Santiago, Chile
SOURCE: Synthetic Communications (1999), 29(12), 2163-2168
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

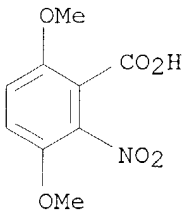


I II III

AB Condensation of 3,6-dimethoxy-2-nitrobenzoyl chloride with L-proline Me ester afforded amide I, which underwent reductive cyclization with iron(II) sulfate and ammonium hydroxide to yield pyrrolobenzodiazepine II. Oxidation of II with (NH4)2Ce(NO3)6 led to the new heterocyclic quinone III in 53% overall yield.

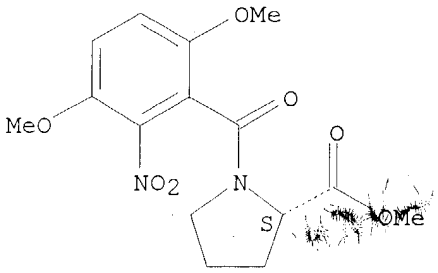
IT **50472-09-8P 50703-23-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn of pyrrolobenzodiazepinequinone via condensation of dimethoxynitrobenzoyl chloride with L-proline Me ester, reductive cyclization, and oxidation)

RN 50472-09-8 HCAPLUS
CN Benzoic acid, 3,6-dimethoxy-2-nitro- (6CI, 9CI) (CA INDEX NAME)



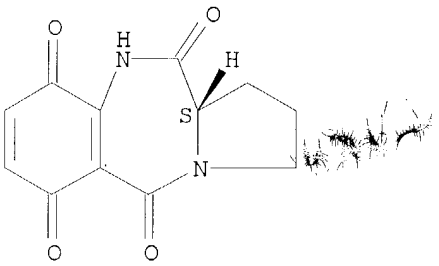
RN 50703-23-6 HCAPLUS
CN L-Proline, 1-(3,6-dimethoxy-2-nitrobenzoyl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



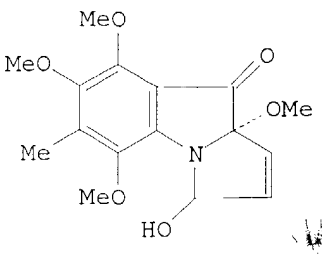
IT **227290-55-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn of pyrrolobenzodiazepinequinone via condensation of dimethoxynitrobenzoyl chloride with L-proline Me ester, reductive cyclization, and oxidation)
RN 227290-55-3 HCAPLUS
CN 1H-Pyrrolo[2,1-c][1,4]benzodiazepine-5,6,9,11(10H,11aH)-tetrone, 2,3-dihydro-, (11aS)- (9CI) (CA INDEX NAME)

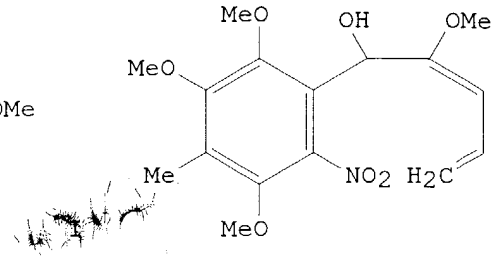
Absolute stereochemistry.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:134108 HCAPLUS
DOCUMENT NUMBER: 120:134108
TITLE: Intramolecular cycloaddition reactions of dienyl nitroso compounds: application to the synthesis of mitomycin K
AUTHOR(S): Benbow, John W.; McClure, Kim F.; Danishefsky, Samuel J.
CORPORATE SOURCE: Dep. Chem., Yale Univ., New Haven, CT, 06511, USA
SOURCE: Journal of the American Chemical Society (1993), 115(26), 12305-14
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:134108
GI





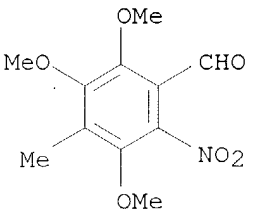
II

AB The total synthesis of mitomycin K has been achieved. The key reaction produced pyrrolo[1,2-a]indole I from dienyl nitrobenzenemethanol II by a process involving two internal photochem. redox transformations and a [4 + 2] cycloaddn.

IT **113727-24-5 141902-69-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(intermediate, preparation of mitomycin K)

RN 113727-24-5 HCAPLUS

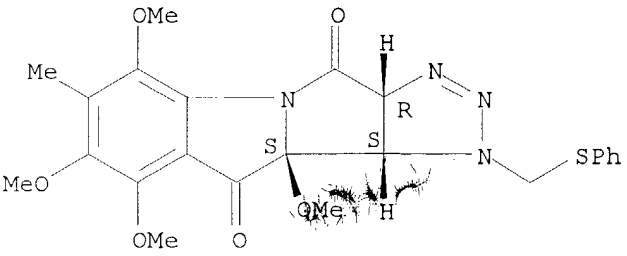
CN Benzaldehyde, 2,3,5-trimethoxy-4-methyl-6-nitro- (9CI) (CA INDEX NAME)



RN 141902-69-4 HCAPLUS

CN 1,2,3-Triazolo[4',5':3,4]pyrrolo[1,2-a]indole-4,10-dione, 1,3a,10a,10b-tetrahydro-6,8,9,10a-tetramethoxy-7-methyl-1-[(phenylthio)methyl]-, (3aα,10aα,10bα)- (9CI) (CA INDEX NAME)

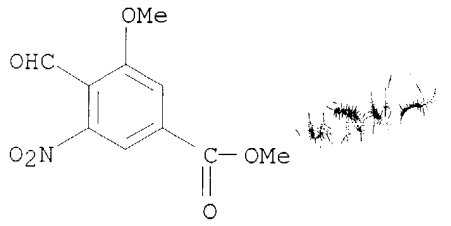
Relative stereochemistry.



IT **136763-83-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and alkylation of)

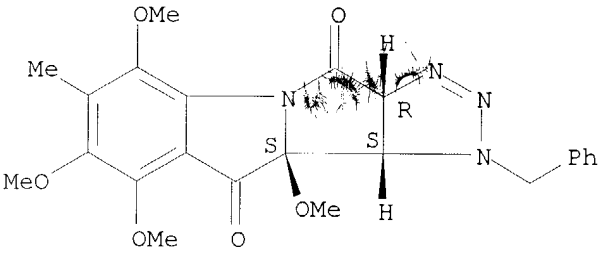
RN 136763-83-2 HCAPLUS

CN Benzoic acid, 4-formyl-3-methoxy-5-nitro-, methyl ester (9CI) (CA INDEX NAME)



IT **152901-51-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and photolysis of)
RN 152901-51-4 HCAPLUS
CN 1,2,3-Triazolo[4',5':3,4]pyrrolo[1,2-a]indole-4,10-dione, 1,3a,10a,10b-tetrahydro-6,8,9,10b-tetramethoxy-7-methyl-1-(phenylmethyl)-, (3aα,10aα,10bα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT **152901-52-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 152901-52-5 HCAPLUS
CN Azirino[2',3':3,4]pyrrolo[1,2-a]indole-2,8-dione, 1,1a,8a,8b-tetrahydro-4,6,7,8a-tetramethoxy-5-methyl-1-(phenylmethyl)-, (1aα,8aα,8bα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.